A comparison among the Homotopy based methods in solving a system of cubic autocatalytic reaction-diffusion equations

***V. Ananthaswamy[1], S. Narmatha[2]**
[1]*PG and Research Department of Mathematics, The Madura College, Madurai Tamil Nadu, India.*
[2]*Department of Mathematics, Lady Doak College, Madurai, Tamil Nadu, India*
**Corresponding author E-mail: ananthu9777@rediffmail.com*

Abstract

The Gray-Scott model of the cubic-autocatalysis with linear decay coupled with diffusion in a one-dimensional reactor is considered. The model is solved using q-Homotopy analysis method, Homotopy analysis method, Homotopy perturbation method and new approach to Homotopy perturbation method. The solutions thus obtained are compared with the numerical solutions obtained using MATLAB. The HAM and the q-HAM seem to best suit this problem. However, since q-HAM has two auxiliary parameters, it is found that q-HAM improves the performance of HAM and hence has more accuracy than the other methods.

Keywords

Gray-Scott model; *q*-Homotopy analysis method; Homotopy analysis method; Homotopy perturbation method; New approach to Homotopy perturbation method; Numerical simulation.

1. Introduction

The main purpose of this paper is to compare the different Homotopy based semi-analytical methods: *q*-Homotopy analysis method, Homotopy analysis method, Homotopy perturbation method and new approach to Homotopy perturbation method with the numerical solution. To exhibit the comparison, we have considered the Gray-Scott model of the cubic-autocatalysis with linear decay coupled with diffusion in a one-dimensional reactor (a reaction diffusion cell) formulated by Marchant [1].

$$a_t = a_{xx} - \beta a b^2 \quad (1)$$

$$b_t = b_{xx} + \beta a b^2 - \beta \gamma b \quad (2)$$

$$a_x = b_x = 0 \text{ at } x = 0 \quad (3)$$

$$a = 1, b = b_0 = k \text{ (say) at } x = 1 \text{ and } t = 0 \quad (4)$$

where a is the dimensionless reactant concentration and b is the dimensionless autocatalyst concentration, β is the measure of the importance of the reaction terms compared with diffusion, while γ is the measure of the importance of the autocatalyst decay compared with the cubic reaction.

2. Homotopy based methods

Various phenomenons in different fields like sciences and engineering can be modelled in the form of linear and non-linear differential equations with appropriate boundary conditions. Such non-linear differential equations do not have an analytic solution, but an approximate analytical solution can be derived using various semi-analytical methods. In this paper, we have solved the mathematical model (eqns. (1) to (4)) using a few of those semi-analytical methods: *q*-Homotopy analysis method [2,3], Homotopy analysis method[4,5] , Homotopy perturbation method [6,7] and new approach to Homotopy perturbation method [8,9]. The basic concept of the *q*-Homotopy analysis method is given in appendix A. The *q*-Homotopy analysis method provides a convenient way to control and adjust the convergence region using the two auxiliary parameters n and q. It should be here noted that the special case of $n=1$ in *q*-HAM gives the HAM and the special case of $h=-1$ in HAM gives the HPM.

3. Semi-analytical solution to the steady state of eqns. (1) to (4) using the different analytical methods

Using *q*- Homotopy analysis method, the solution is

$$a=\frac{1}{24n^2}\left(\begin{array}{l}2\left(\frac{\beta(x^2-5)k^2}{2}+(-x^2+5)\beta k-6+\gamma(x^2-5)\beta\right)k^2\beta(x^2-1)h^2\\-24k^2n\beta(x^2-1)h+24n^2\end{array}\right)\tag{5}$$

$$b=\frac{1}{24n^2}\left(\left(\begin{array}{l}((x^2+1)(-k^3+\gamma^2-3\gamma k+2k^2)\beta-12\gamma+12k)(x^2-1)\beta h^2\\-6(x+1)\beta((-k^3+\gamma^2-3\gamma k+2k^2)\beta+4n(-k+\gamma))(x-1)h+24n^2\end{array}\right)k\right)\tag{6}$$

Using Homotopy analysis method, the approximate analytical expressions of the eqns. (1) – (4) are as follows:

$$a=\frac{1}{24}\left(\begin{array}{l}2\left(\frac{\beta(x^2-5)k^2}{2}+(-x^2+5)\beta k-6+\gamma(x^2-5)\beta\right)k^2\beta(x^2-1)h^2\\-24k^2\beta(x^2-1)h+24\end{array}\right)\tag{7}$$

$$b=\frac{1}{24}\left(\left(\begin{array}{l}((x^2+1)(-k^3+\gamma^2-3\gamma k+2k^2)\beta-12\gamma+12k)(x^2-1)\beta h^2\\-6(x+1)\beta((-k^3+\gamma^2-3\gamma k+2k^2)\beta+4(-k+\gamma))(x-1)h+24\end{array}\right)k\right)\tag{8}$$

Using Homotopy perturbation method, the approximate analytical expressions of the eqns. (1) – (4) are as follows:

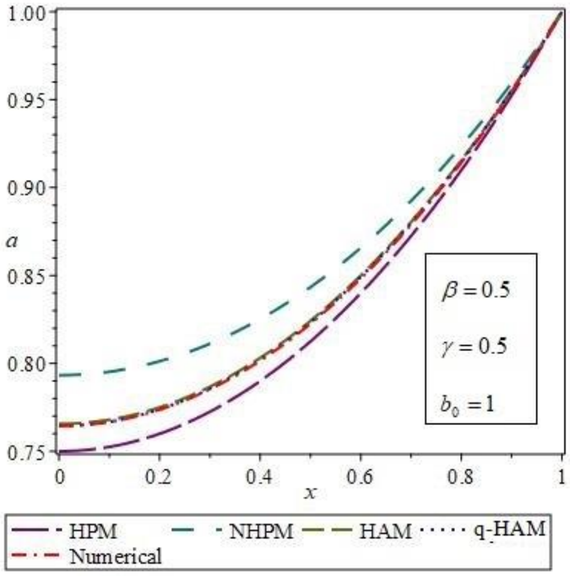
$$a=\frac{1}{24}\left(\begin{array}{l}2\left(\frac{\beta(x^2-5)k^2}{2}+(-x^2+5)\beta k-6+\gamma(x^2-5)\beta\right)k^2\beta(x^2-1)\\+24k^2\beta(x^2-1)+24\end{array}\right)\tag{9}$$

$$b=\frac{1}{24}\left(\left(\begin{array}{l}((x^2+1)(-k^3+\gamma^2-3\gamma k+2k^2)\beta-12\gamma+12k)(x^2-1)\beta\\-6(x+1)\beta((-k^3+\gamma^2-3\gamma k+2k^2)\beta-4(-k+\gamma))(x-1)+24\end{array}\right)k\right)\tag{10}$$

Using new approach to Homotopy perturbation method, the approximate analytical expressions of the eqns. (1) – (4) are as follows:

$$a = \frac{\cosh\sqrt{\beta}kx}{\cosh\sqrt{\beta}k} \tag{11}$$

$$b = \frac{\gamma - k}{\gamma}\frac{\cosh\sqrt{\beta\gamma}x}{\cosh\sqrt{\beta\gamma}} + \frac{k^2}{\gamma} \tag{12}$$



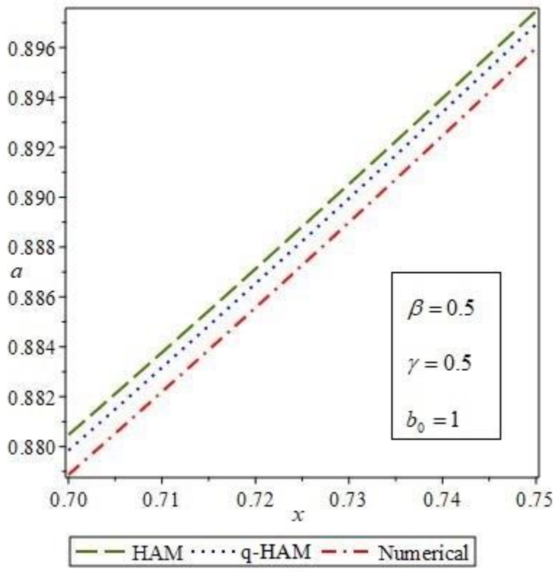
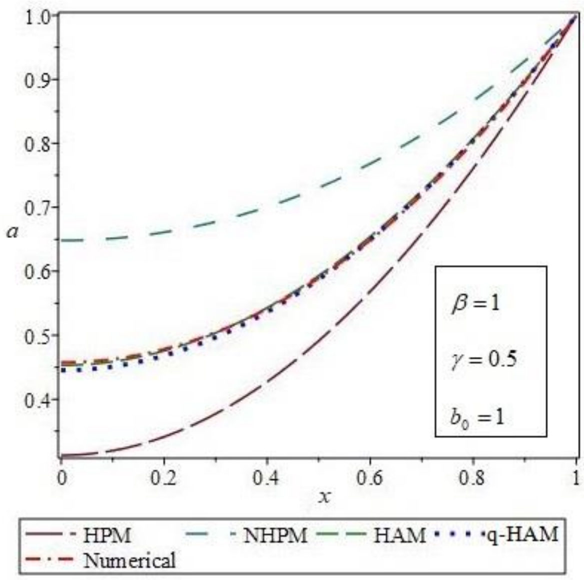


Fig1(a). **Fig1(b).**

Fig.1: Comparison among the approximate analytical solutions obtained using *q*-HAM, HAM, HPM and NHPM with the numerical solution obtained using MATLAB. For HAM, the value of h is -0.72, while for q-HAM, $n=10, h=-7.3$.



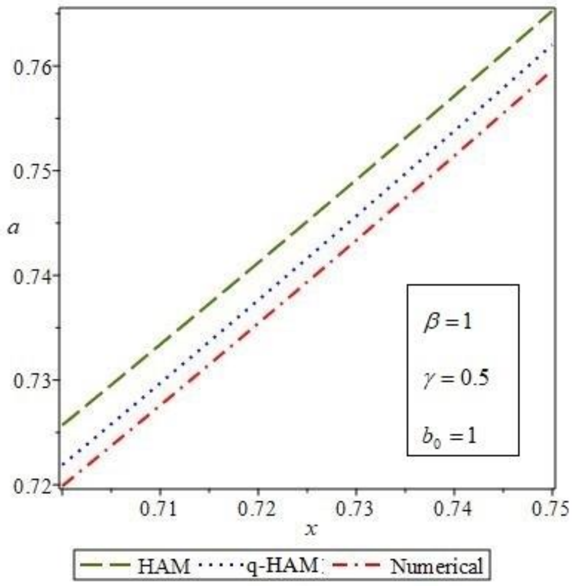


Fig.2(a). **Fig.2(b).**

Fig.2: Comparison among the approximate analytical solutions obtained using q-HAM, HAM, HPM and NHPM with the numerical solution obtained using MATLAB. For HAM, the value of h is -0.714, while for *q*-HAM, $n=10, h=-7$.

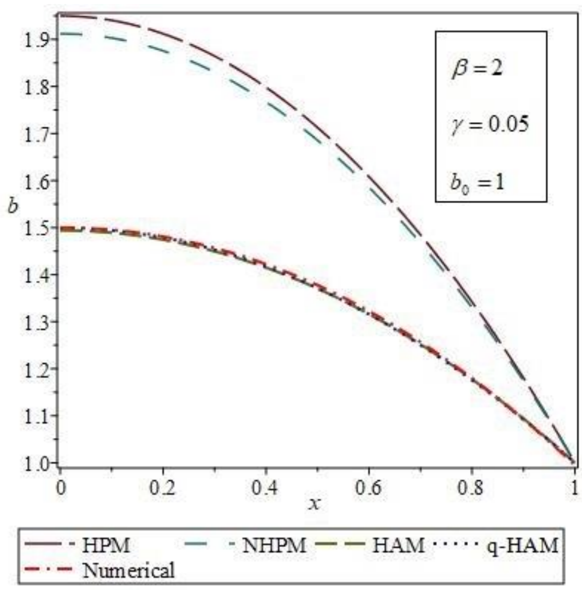


Fig3(a).

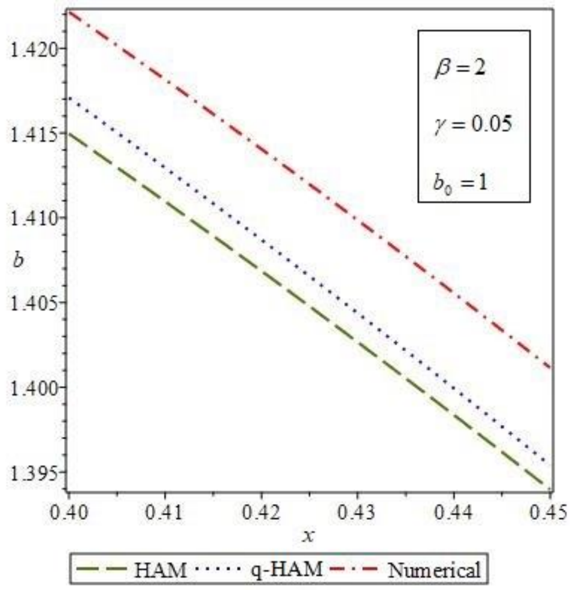


Fig3(b).

Fig.3: Comparison among the approximate analytical solutions obtained using q-HAM, HAM, HPM and NHPM with the numerical solution obtained using MATLAB. For HAM, the value of h is -0.52, while for q-HAM, $n=10, h=-3.48$.

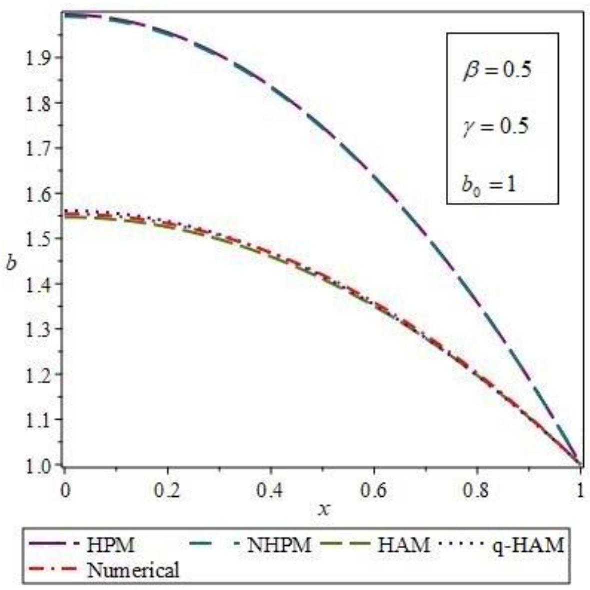


Fig4(a).

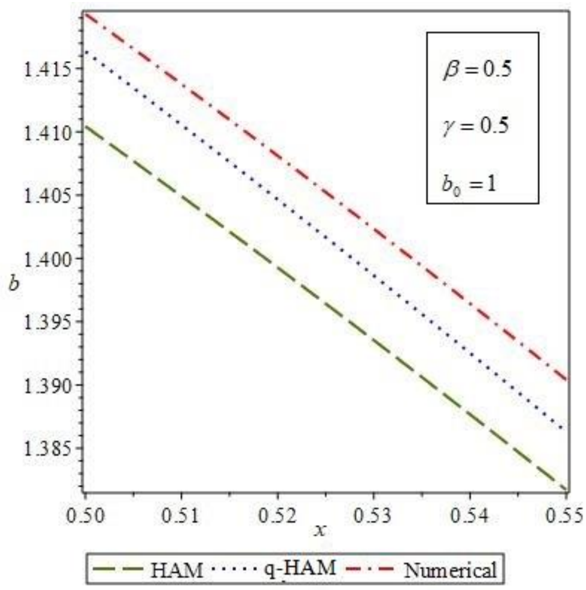


Fig4(b).

Fig.4: Comparison among the approximate analytical solutions obtained using q-HAM, HAM, HPM and NHPM with the numerical solution obtained using MATLAB. For HAM, the value of h is -0.55, while for q-HAM, $n=10, h=-3.6$.

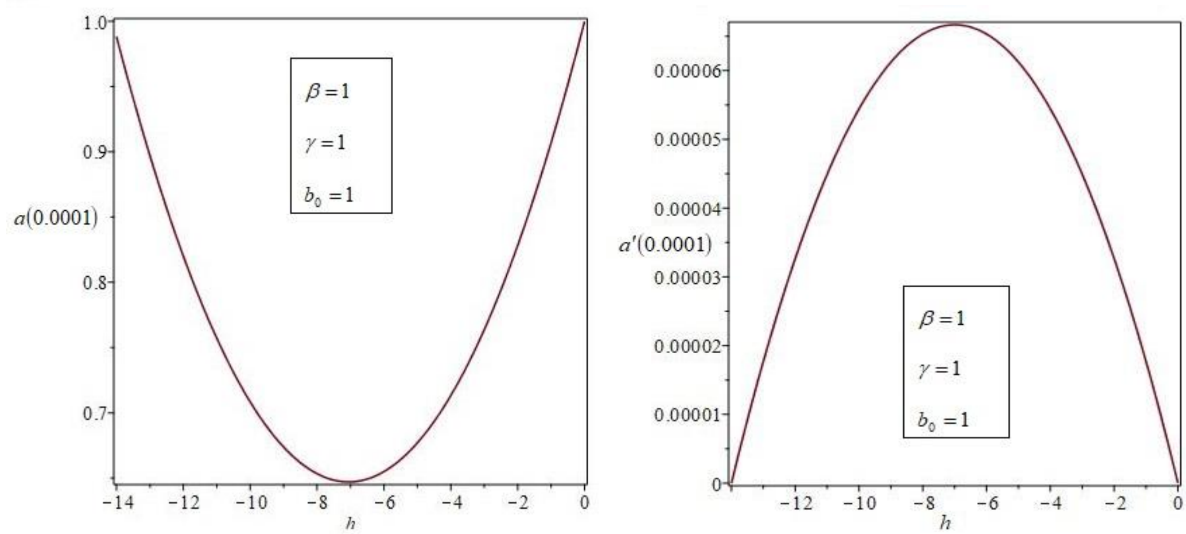


Fig.5: h curves are plotted to indicate the convergence of the analytical solution obtained using q-HAM for $n = 10$.

Table 1: Percentages of deviation of the derived analytical solutions from the simulation result in Fig1.

x	Dimensionless reactant concentration a								
	Numerical Simulation	**q-HAM**	**Absolute error %**	**HAM**	**Absolute error %**	**HPM**	**Absolute error %**	**NHPM**	**Absolute error %**
0	0.76442	0.7644	0	0.765625	0.16	0.75	1.89	0.7932781823	3.78
0.2	0.7736788956	0.773824	0.02	0.775	0.17	0.76	1.77	0.8012241943	3.56
0.4	0.8015503311	0.802096	0.07	0.803125	0.20	0.79	1.44	0.8252214149	2.95
0.6	0.8483004989	0.849216	0.11	0.85	0.20	0.84	0.98	0.8657505902	2.06
0.8	0.9143125195	0.915184	0.10	0.915625	0.14	0.91	0.47	0.9236236550	1.02
1	1	1	0	1	0	1	0	1	0
Average absolute error %			**0.05**		**0.14**		**1.09**		**2.23**

Table 2: Percentages of deviation of the derived analytical solutions from the simulation result in Fig.2.

x	Dimensionless reactant concentration a								
	Numerical Simulation	**q-HAM**	**Absolute error %**	**HAM**	**Absolute error %**	**HPM**	**Absolute error %**	**NHPM**	**Absolute error %**
0	0.45744	0.4553112500	0.47	0.453125	0.94	0.3125	31.69	0.6480542735	41.67
0.2	0.4782835902	0.4762329062	0.43	0.4757056	0.54	0.34144	28.61	0.6610586204	38.21
0.4	0.5415604311	0.5366308218	0.91	0.5430946	0.28	0.42754	21.05	0.7005935704	29.37

0.6	0.6490406190	0.6494038374	0.06	0.6542336	0.80	0.56864	12.39	0.7682458012	18.37
0.8	0.8021555641	0.8047166874	0.32	0.8073586	0.65	0.76114	5.11	0.8667304325	8.05
1	1	1	0	1	0	1	0	1	0
Average absolute error %			**0.36**		**0.54**		**16.48**		**22.61**

Table 3: Percentages of deviation of the derived analytical solutions from the simulation result in Fig3.

x	**Dimensionless autocatalyst concentration** *b*								
	Numerical Simulation	**q-HAM**	**Absolute error %**	**HAM**	**Absolute error %**	**HPM**	**Absolute error %**	**NHPM**	**Absolute error %**
0	1.5	1.499277340	0.05	1.494	0.4	1.95	30	1.911963661	27.46
0.2	1.480729908	1.478645503	0.14	1.47424	0.44	1.912	29.13	1.875775523	26.68
0.4	1.422144206	1.417080364	0.36	1.41496	0.51	1.798	26.43	1.767066322	24.25
0.6	1.322388189	1.315573037	0.52	1.31616	0.47	1.608	21.60	1.585401087	19.89
0.8	1.179890150	1.175775382	0.35	1.17784	0.17	1.342	13.74	1.330052878	12.73
1	1	1	0	1	0	1	0	1	0
Average absolute error %			**0.24**		**0.33**		**20.15**		**18.50**

Table 4: . Percentages of deviation of the derived analytical solutions from the simulation result in Fig.4.

x	**Dimensionless autocatalyst concentration** *b*								
	Numerical Simulation	**q-HAM**	**Absolute error %**	**HAM**	**Absolute error %**	**HPM**	**Absolute error %**	**NHPM**	**Absolute error %**
0	1.5544	1.561374141	0.45	1.54725	0.46	1.995	28.34	1.99087102	28.08
0.2	1.533124824	1.537960313	0.32	1.52536	0.51	1.9552	27.53	1.951267698	27.27
0.4	1.468486835	1.468198259	0.02	1.45969	0.60	1.8358	25.01	1.832442522	24.78
0.6	1.358587447	1.353526274	0.37	1.35024	0.61	1.6368	20.48	1.634347796	20.30
0.8	1.202001348	1.196341514	0.47	1.19701	0.42	1.3582	13.00	1.356903691	12.89
1	1	1	0	1	0	1	0	1	0
Average absolute error %			**0.27**		**0.43**		**19.06**		**18.89**

5. Results and discussions

The steady state analytical expressions for the dimensionless concentration of the reactant and autocatalyst have been derived using the four Homotopy based methods. The solutions derived using *q*-HAM and NHPM are elaborated in Appendix *B* and *C* respectively. The four derived analytical expressions along with the numerical solution obtained using MATLAB have been plotted in Figs. 1 to 4. The corresponding deviation percentages are tabulated in tables 1 to 4. The MATLAB program is given in Appendix D.

From Figs. 1 to 4 and Tables 1 to 4, we observe that though HAM and *q*-HAM are both best suitable for solving this mathematical model, *q*-HAM gives a closer approximation to the numerical solution that HAM. The *h*-curves for *q*- HAM are given in Fig.5. The figure clearly indicates that the valid region of *h* for $n=10$ is -7.5 to -6.5.

6. Conclusion

The main purpose of this paper is to compare the four methods and find out the best choice for this problem. Consequently, the four methods were applied and the corresponding analytical solutions were derived. We hence noted that, for this problem the *q*-HAM improves the performance of HAM and has more accuracy than the other methods.

Appendix: A

To illustrate the basic ideas of the *q*-Homotopy analysis method (*q*-HAM), consider the following non-linear boundary value problem [2,3]

$$\left.\begin{aligned} &N[u(t)]=0;\ t\in\eta \\ &B\left(u(t),\frac{du}{dt}\right)=0;\ t\in\gamma \end{aligned}\right\} \tag{A.1}$$

where $u(t)$ defined over the region η is the function to be solved under the boundary constraints *B* defined over the boundary γ of η.

The *q*- Homotopy analysis technique defines a Homotopy $\phi(t,q):R\times\left[0,\frac{1}{n}\right]\to R$ so that

$$H(\phi,q)=(1-nq)\left[L(\phi(t,q))-L(u_0)\right]-qhN[\phi(t,q)]=0 \tag{A.2}$$

where $q\in\left[0,\frac{1}{n}\right], n\geq 1$ denotes the so-called embedded parameter, $h\neq 0$ is an auxiliary parameter, *L* is a suitable auxiliary linear operator, u_0 is an initial approximation of equation (A.1) satisfying exactly the boundary conditions. It is obvious from the eqn. (A.2) that

$$H(\phi,0)=\left[L(\phi(t,q))-L(u_0)\right],\ H\left(\phi,\frac{1}{n}\right)=\frac{h}{n}N\left[\phi\left(t,\frac{1}{n}\right)\right]$$

The solution of eqn. (A.2) exists as a power series in q.

Hence, $\phi(t,q)=u_0(t)+qu_1(t)+q^2u_2(t)+...$ (A.3)

The appropriate solutions of the coefficients $u_k(t)$ in an eqn. (A.3) can be found from the Homotopy deformation equations. Hence the approximate solution of the eqn. (A.1) can be obtained as

$u(t) = \lim_{q \to \frac{1}{n}} \phi(t,q) = \sum_{k=0}^{\infty} u_k(t) \left(\frac{1}{n}\right)^k$. It was found that the auxiliary parameters h and n can adjust and control the convergence region and the rate of the Homotopy series solutions.

Appendix: B

In this appendix, we have derived the steady state solution of eqns. (1) to (4) using q-HAM. The eqns. (1) and (2) in steady state become

$$\frac{d^2a}{dx^2} - \beta ab^2 = 0 \tag{B.1}$$

$$\frac{d^2b}{dx^2} + \beta ab^2 - \beta\gamma b = 0 \tag{B.2}$$

We construct the q-Homotopy for eqns. (B.1) and (B.2) as follows:

$$(1-nq)\left[\frac{d^2a}{dx^2}\right] = qh\left[\frac{d^2a}{dx^2} - \beta ab^2\right] \tag{B.3}$$

$$(1-nq)\left[\frac{d^2b}{dx^2}\right] = qh\left[\frac{d^2b}{dx^2} + \beta ab^2 - \beta\gamma b\right] \tag{B.4}$$

Let the approximate solution of the eqns.(B.3) and (B.4) be

$$a = a_o + a_1 q + a_2 q^2 + ... \tag{B.5}$$

$$b = b_o + b_1 q + b_2 q^2 + ... \tag{B.6}$$

Substituting the eqns. (B.5) and (B.6) in eqns. (B.3) and (B.4), and equating the coefficients of q^0, q^1 and q^2, we get

$$q^0: \quad \frac{d^2a_o}{dx^2} = 0 \tag{B.7}$$

$$\frac{d^2b_o}{dx^2} = 0 \tag{B.8}$$

$$q^1: \quad \frac{d^2a_1}{dx^2} - n\frac{d^2a_0}{dx^2} = h\left[\frac{d^2a_0}{dx^2} - \beta a_0 {b_0}^2\right] \tag{B.9}$$

$$\frac{d^2b_1}{dx^2} - n\frac{d^2b_0}{dx^2} = h\left[\frac{d^2b_0}{dx^2} + \beta a_0 {b_0}^2 - \beta\gamma b_0\right] \tag{B.10}$$

$$q^2: \quad \frac{d^2a_2}{dx^2} - n\frac{d^2a_1}{dx^2} = h\left[\frac{d^2a_1}{dx^2} - \beta\left(2a_0 b_0 b_1 + a_1 {b_0}^2\right)\right] \tag{B.11}$$

$$\frac{d^2b_2}{dx^2} - n\frac{d^2b_1}{dx^2} = h\left[\frac{d^2b_1}{dx^2} + \beta\left(2a_0 b_0 b_1 + a_1 {b_0}^2\right) - \beta\gamma b_1\right] \tag{B.12}$$

The initial approximations are as follows:

$$\text{At } x = 0, \quad \frac{da_i}{dx} = 0,\ i = 0,1,2,3,... \tag{B.13}$$

$$\frac{db_i}{dx} = 0,\ i = 0,1,2,3,... \tag{B.14}$$

At $x = 1$, $$a_o = 1;\ a_i = 0,\ i = 2,3,4,... \tag{B.15}$$

$$b_o = k;\ b_i = 0,\ i = 2,3,4,... \tag{B.16}$$

Solving eqns. (B.7) to (B.16), we get

$$a_0 = 1,\ b_0 = k \tag{B.17}$$

$$a_1 = \frac{h\beta k^2(1-x^2)}{2},\ b_1 = \frac{h\beta k(k-\gamma)(x^2-1)}{2} \tag{B.18}$$

$$a_2 = \left[\frac{\left(\frac{h\beta^2 k^4}{2} - h\beta^2 k^2(k-\gamma)\right)\ h\ (x^4-1)}{12}\right] + \left[\frac{\left(-\frac{h^2 p^2 k^4}{2} + h^2 p^2 k^2(k-\gamma) - h^2\beta\ k^2 - h\beta\ k^2 n\right)(x^2-1)}{2}\right] \tag{B.19}$$

$$b_2 = \frac{1}{12}\left[\left(-\frac{h^2\beta^2 k^4}{2} + h^2\beta^2 k^2(k-\gamma) - \frac{h^2\beta^2\gamma k(k-\gamma)}{2}\right)(x^4-1)\right] + \frac{1}{2}\left(h^2\left(\begin{array}{l}(\beta k^2 - \beta\gamma k) + [n h\ (\beta k^2 - \beta\gamma k)] + \left[\frac{h\beta^2 k^4}{2}\right] - [h\beta^2 k^2(k-\gamma)] \\ + \left[\frac{\beta^2\gamma h k(k-\gamma)}{2}\right]\end{array}\right)(x^2-1)\right) \tag{B.20}$$

Hence we get the approximate solutions are as follows:

$$a = \lim_{q\to\frac{1}{n}}(a_o + a_1 q + a_2 q^2 +) \approx a_0 + \frac{a_1}{n} + \frac{a_2}{n^2}$$

$$= \frac{1}{24n^2}\left(\begin{array}{l}2\left(\frac{\beta(x^2-5)k^2}{2} + (-x^2+5)\beta k - 6 + \gamma(x^2-5)\beta\right)k^2\beta(x^2-1)h^2 \\ -24k^2 n\beta(x^2-1)h + 24n^2\end{array}\right) \tag{B.21}$$

$$b = \lim_{q\to\frac{1}{n}}(b_o + b_1 q + b_2 q^2 + ...) \approx b_0 + \frac{b_1}{n} + \frac{b_2}{n^2}$$

$$= \frac{1}{24n^2}\left(\left(\begin{array}{l}((x^2+1)(-k^3+\gamma^2-3\gamma k+2k^2)\beta - 12\gamma + 12k)(x^2-1)\beta h^2 \\ -6(x+1)\beta((-k^3+\gamma^2-3\gamma k+2k^2)\beta + 4n(-k+\gamma))(x-1)h + 24n^2\end{array}\right)k\right) \tag{B.22}$$

Appendix: C

In this appendix, we derive the steady state solution to eqns. (1) to (4) using new Homotopy perturbation method

The eqns. (1) and (2) in steady state become

$$\frac{d^2a}{dx^2} - \beta ab^2 = 0 \tag{C.1}$$

$$\frac{d^2b}{dx^2} + \beta ab^2 - \beta\gamma\, b = 0 \tag{C.2}$$

We construct the Homotopy for the eqns. (C.1) and (C.2) as follows:

$$(1-p)\left[\frac{d^2a}{dx^2} - \beta ak^2\right] + p\left[\frac{d^2a}{dx^2} - \beta ab^2\right] = 0 \tag{C.3}$$

$$(1-p)\left[\frac{d^2b}{dx^2} + \beta(1)(k)(k) - \beta\gamma b\right] + p\left[\frac{d^2b}{dx^2} + \beta ab^2 - \beta\gamma b\right] = 0 \tag{C.4}$$

Let the approximate solutions of (C.3) and (C.4) be

$$a = a_o + a_1 p + a_2 p^2 + ... \tag{C.5}$$

$$b = b_o + b_1 p + b_2 p^2 + ... \tag{C.6}$$

Substituting eqns. (C.5) and (C.6) in eqns. (C.3) and (C.4), and equating the coefficients of p^0 we get

$$\frac{d^2a_0}{dx^2} - \beta a_0 k^2 = 0 \tag{C.7}$$

$$\frac{d^2b_0}{dx^2} + \beta(1)(k)(k) - \beta\gamma b_0 = 0 \tag{C.8}$$

The initial approximations are as follows:

At $x = 0$, $$\frac{da_i}{dx} = 0,\ i = 0,1,2,3,\ldots \tag{C.9}$$

$$\frac{db_i}{dx} = 0,\ i = 0,1,2,3,\ldots \tag{C.10}$$

At $x = 1$, $$a_o = 1\ ;\ a_i = 0,\ i = 2,3,4,\ldots \tag{C.11}$$

$$b_o = k\ ;\ b_i = 0,\ i = 2,3,4,\ldots \tag{C.12}$$

Solving the eqns. (C.7) and (C.8) using eqns. (C.9) to (C.12), we get the following results

$$a_0 = \frac{\cosh\sqrt{\beta}kx}{\cosh\sqrt{\beta}k}$$

$$b_0 = \frac{\gamma - k}{\gamma}\frac{\cosh\sqrt{\beta\gamma}x}{\cosh\sqrt{\beta\gamma}} + \frac{k^2}{\gamma}$$

Hence, $a \approx \dfrac{\cosh\sqrt{\beta}kx}{\cosh\sqrt{\beta}k},\ b \approx \dfrac{\gamma - k}{\gamma}\dfrac{\cosh\sqrt{\beta\gamma}x}{\cosh\sqrt{\beta\gamma}} + \dfrac{k^2}{\gamma}.$

Appendix: D

Nomenclature

Symbols	Meaning
a	dimensionless concentration of the reactant
b	dimensionless concentration of the autocatalyst
β	measure of the importance of the reaction terms
γ	measure of the importance of the autocatalyst decay

Appendix: E

MATLAB program to find the numerical solution of eqns. (1)-(4)

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function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,0.5);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,2)')
%------------------------------------------
figure
plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
ylabel('u2(x,2)')
% ----------------------------------------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1; 1] .* DuDx;
g=0.05;
b=2;
F=(-b*(u(1)*u(2))*u(2));
F1=(b*u(1)*u(2)*u(2)-b*g*u(2));
s=[F; F1];
% ----------------------------------------
function u0 = pdex4ic(x);
u0 = [1; 1];
% ----------------------------------------
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = [0;0];
```

```
ql = [1;1];
pr = [ur(1)-1;ur(2)-0.5];
qr = [0;0];
```

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